

False negatives = C/(A+C)

False positives = B/(B+D)

Sensitivity = A/(A+C)

Efficiency = D/(D+B)

Predicted hit reliability = A/(A+B)

Predicted no-hit reliability = D/(D+C)

Overall reliability = (D+A)/(A+B+C+D)

Figure 3-1. Calculation of reliability parameters

| Figure 4-1  | Correlations that has | e a significant Pearso  | n's correlation coefficient  |
|-------------|-----------------------|-------------------------|------------------------------|
| riguic 4-1. | Conciations that have | c a significant i carso | ii s corretation coefficient |

| Figure 4-1.            | Correlations that have a signifi                           | icant Pearson's       | con     | elatio          | n coe                        | fficien           | nt          |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|------------------------|--|-----------------------|---------|-----------------|------------------------------|-------------------|-------------|--------------|--------------------|------------|---|----------|------------|-------------------------|-------------|--------------|----------------------|-------------------------------|----------|------|------|----------|-------|-------|---------|------|--------------|-----------------|------------------------------|--------|----------|------------|-----------------------|-----------------------------------|---------|--------|-------------------------------------|------------------|------------------------------------|-----------|-----------------------------------|--|
|                        |  | onal                  |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               | ganic    |      |      |          |       |       |         |      |              |                 | Organic                      |        | n        |            |                       |                                   |         | s      |                                     |                  |                                    |           |                                   |  |
|                        |  | ventio                |         | Щ               |                              |                   |             |              |                    |            |   | H        | E          |                         |             | Pesticides   | . Organ              | 1                             | -        |      |      |          | :     |       |         |      | o.           |                 | Organotin                    |        | sam      |            |                       | icide                             |         |        |                                     | lol              |                                    | Phthalate |                                   |  |
|                        |  | Con,                  |         |                 |                              |                   | НРАН        |              |                    |            |   |          |            | LPAH                    | 4           |              | PAH sum              | Pesti                         | Misc     |      |      |          |       | Metal |         |      |              |                 | Misc.                        |        | Orga     |            | PAH                   |                                   |         | Pesti  |                                     |                  |                                    | Phenol    |                                   | Phth   |
|                        |  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 | ਰ ਓ                          |        |          |            |                       | ane                               | ıne     | ane    |                                     |                  |                                    |           | 9                                 |  |
|                        |  |                       |         |                 |                              |                   |             |              | e                  |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 | Total Dioxin Furans (calc'd) |        |          |            | el-Range Hydrocarbons | ohex                              | hexa    | hex    | <del>©</del>                        |                  | (c,q)                              |           | enol<br>s(2-ethylhexyl) phthalate |  |
|                        |  |                       |         | ne              | thene                        | ene               | ene         | cene         | pyre               | 1 5        | ene   |          |            |                         |             | :            | (p, c                | ਰੇ                            |          |      |      |          |       |       |         |      |              | e               | o) sun                       |        |          |            | droca                 | cvc                               | ycloh   | cycle  | calc                                | 1 1              | ਰ                                  | 0-1       | pht                               | alate  |
|                        |  |                       |         | race            |                              | eryl              | rant        | nthra        | c,d)py             |            | hthal                                       | မ        | ene        |                         |             |              | ca ca                | calc                          | _        |      |      |          |       |       |         |      |              | enze            | Fura                         |        | _        |            | Hy                    | l of                              | chloroc | loro   | r<br>ane (                          | calc             | Ifan                               |           | (lxyl)                            | phth   |
|                        |  | _   _   _             |         | enzo(a)anthrace | izo(a)pyrene<br>izo(b)fluora | zo(g,h,i)perylene | ene         | ız(a,h)anthı | hene<br>,2,3       |            | 10tal HFAHS (calc d)<br>2-Methylnaphthalene | then     | naphthylei | e                       | lene        | Phenanthrene | Fotal LPAHs (calc'd) | Total PAHs (calc'd) Carbazole | nzofuran | 2    | ,    | _        |       |       |         |      |              | xachlorobenzene | tal Dioxin Furans            | .      | outyltin | ibutyltin  | ange                  | Aldrin<br>ulnha-Hexachlorocyclohe | cachl   | xachlo | thoxychlor<br>al Chlordane (calc'd) | al DDTs (calc'd) | otal Endosulfan (c<br>Methylphenol | orop      | nylhe                             | Butyl benzyl phthalate<br>Di-n-butyl phthalate |
|                        |  | Fines (%) TOC Ammonia | ide     | zo(a)           | zo(a,<br>zo(b)               | g)oz              | zo(k)       | )zua         | ranther<br>no(1,2, | ine l      | ethy  | enaphthe | naph       | Antinracene<br>Fluorene | Vaphthalene | ant          |                      | II PA                         | ozua     | mony | nic  | Chromium | opper | _   ř | sel sel | nium | . l d        | achle           | I Di                         | ıtylti | inqoi    | ributyltin | el-R                  | H.                                | -Неха   | a-Hex  | hoxy<br>II Ch                       |                  | I En                               | achlor    | nol<br>2-etł                      | /l be  |
| Group                  | Chemical   | Fine                  | Sulfide | Ben             | Ben                          | Ben               | Ben<br>Chr. | Dibe         | Eluc<br>Inde       | Pyre       | 1012<br>2-M                                 | Ace      | Ace        | And                     | Nap         | Pher         | Tota                 | Cart Ots                      | Dibe     | Anti | Arse | G G      | Cop   | Lead  | Nic.    | Sele | Silv<br>Zinc | Hex             | Tota                         | Dib    | Mor      |            | Dies                  | Aldrin<br>alnha-F                 | beta    | delta  | Met<br>Tota                         | Tota             | Tota<br>4-M                        | Pent      | Pher<br>Bis(                      | Buty<br>Di-n                                   |
| Conventional           | Fines (%) TOC  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Ammonia  | -                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Sulfide  |                       | _       |                 |                              |                   |             |              |                    |            | _   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| НРАН                   | Benzo(a)anthracene<br>Benzo(a)pyrene                       | -                     |         | X<br>X          |                              |                   |             |              | x x<br>x x         |            |   |          | X X X      |                         |             | X X          |                      |                               | X        |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Benzo(b)fluoranthene                                       |                       | - 1     | x x             |                              |                   |             |              | x x                |            |   |          | x x        |                         |             | x 2          |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Benzo(g,h,i)perylene<br>Benzo(k)fluoranthene               | 1                     | - 1     | x x             |                              |                   | x x         |              |                    | X X        |   |          | X X        |                         |             | X 2          |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Chrysene   | †                     | - 1     |                 | X                            | X                 |             | X            | x x<br>x x         | X X        |   |          | X X X      |                         |             | X X          |                      | XX                            |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Dibenz(a,h)anthracene                                      |                       | - 1     |                 |                              |                   | x x         |              | x x                |            |   |          | x x        |                         |             |              |                      | x x                           |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Fluoranthene<br>Indeno(1,2,3-c,d)pyrene                    | 1                     | - 1     |                 |                              |                   | x x x x     |              |                    | X X<br>X X |   |          | X X X      |                         |             | X X          |                      |                               | X        |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Pyrene   | ]                     | - 1     |                 |                              |                   | x x         |              |                    | Х          |   |          | x x        |                         |             | x 2          |                      |                               | x        |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| HPAH sum<br>LPAH       | Total HPAHs (calc'd) 2-Methylnaphthalene                   |                       |         | X X             | X                            | X                 | x x         | X            | x x                | X          |   |          | x x x x    |                         | v           | X X          |                      |                               | X        |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| LFAII                  | Acenaphthene   |                       |         | x               |                              |                   | x           |              | X                  | x x        | x   | А        |            | X                       |             | X X          |                      |                               | X<br>X   |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Acenaphthylene   |                       |         |                 |                              |                   | x x         |              |                    | X X        |   |          | X          |                         |             | x 2          |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Anthracene<br>Fluorene                                     | -                     |         | x x x           |                              |                   | x x x       |              | x x<br>x           | X X<br>X X |   | X<br>X   | X<br>X     | X                       |             | X X          |                      | x x                           | X<br>X   |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Naphthalene  |                       |         |                 |                              |                   |             | ••           | •                  |            | x   |          | •          | -                       |             |              | x .                  | •                             |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Phenanthrene<br>Total LPAHs (calc'd)                       |                       |         | x x             | X                            | X                 |             |              | x x                |            |   |          |            |                         |             |              | x x                  |                               | X        |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| PAH sum                | Total PAHs (calc'd)  | -                     |         | x x             | X                            | X<br>X            | x x x       | X<br>X       |                    | X X<br>X X |   |          |            |                         | X           | x 2          | X X                  | _                             | X<br>X   |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| Pesticide              | Carbazole  | ]                     |         | X               | X                            |                   | x x         |              |                    | x x        |   |          | X          |                         |             |              | X                    | -                             |          | ,    |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| Misc. organic<br>Metal | Dibenzofuran<br>Aluminum                                   | -                     |         | X               |                              |                   | X           |              | X                  | X X        | X   | Х        | Х          | X                       |             | X 2          | X X                  | X.                            |          |      |      |          |       |       |         |      |              | 1               |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Antimony   |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Arsenic<br>Cadmium   |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Chromium   | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Copper   | ]                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Lead<br>Mercury  | -                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Nickel   |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Selenium   | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Silver<br>Zinc   | †                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| Misc. organic          | Hexachlorobenzene  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Total dioxins/furans (calc'd) Total PCBs Aroclors (calc'd) | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| Organotin              | Dibutyltin   |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        | X        |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Monobutyltin<br>Tetrabutyltin                              | -                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              | X      |          | v          |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Tributyltin  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        | х        |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| PAH sum                | Diesel-Range Hydrocarbons                                  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            | $\Box$                |                                   |         |        |                                     |                  | х                                  |           |                                   |  |
| Pesticide              | Aldrin alpha-Hexachlorocyclohexane                         | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | beta-Hexachlorocyclohexane                                 | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | delta-Hexachlorocyclohexane<br>Methoxychlor                | -                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Total chlordane (calc'd)                                   | <u> </u>              |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Total DDTs (calc'd)  |                       |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
| Phenol                 | Total endosulfan (calc'd) 4-Methylphenol                   | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            | х                     |                                   |         |        |                                     |                  |                                    | X         | $\neg$                            | I  |
|                        | Pentachlorophenol  | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  | x                                  |           |                                   | I  |
| Phthalate              | Phenol<br>Bis(2-ethylhexyl) phthalate                      | -                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           | +                                 |  |
| riiiiaiate             | Butyl benzyl phthalate                                     | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |
|                        | Di-n-butyl phthalate                                       | 1                     |         |                 |                              |                   |             |              |                    |            |   |          |            |                         |             |              |                      |                               |          |      |      |          |       |       |         |      |              |                 |                              |        |          |            |                       |                                   |         |        |                                     |                  |                                    |           |                                   |  |

This figure summarizes the correlations that have a significant Pearson's correlation coefficient (minimum r: 0.9; maximum p value: 0.01).

Note: Only the upper triangle of the original matrix was filled; see intersections of rows and columns for important correlations with each chemical.

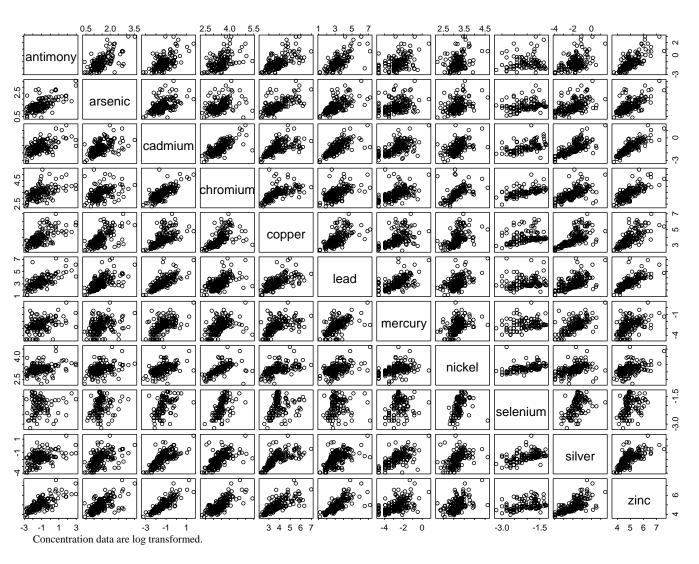
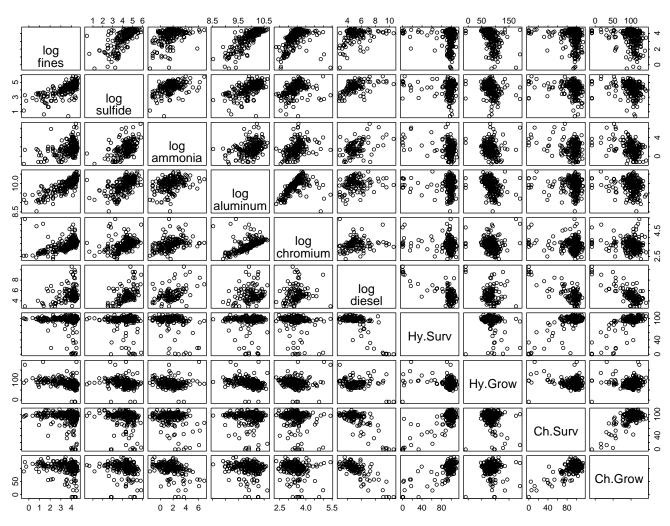


Figure 4-2. Pairwise scatter plots for metals



Biological endpoints were control adjusted; skewed chemical analytes were natural-log-transformed.

Figure 4-3. Pairwise scatter plots for biological endpoints and selected chemical and physical analytes

## DO NOT QUOTE OR CITE

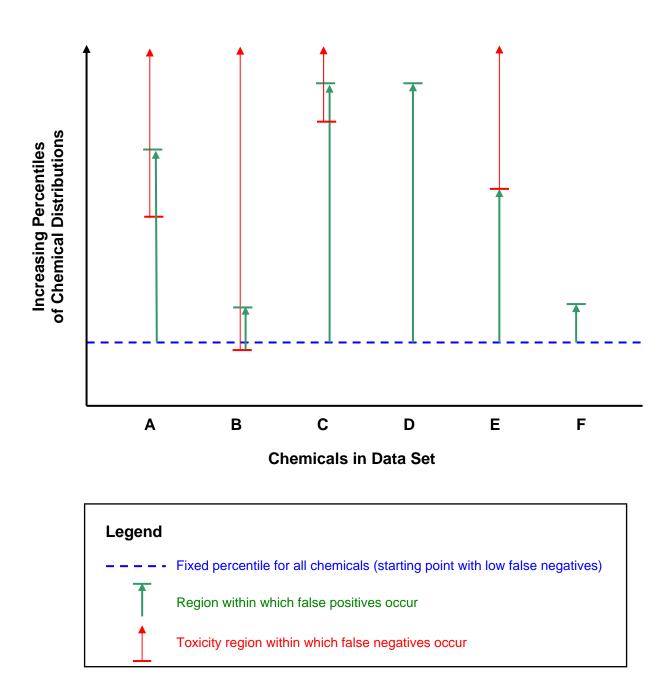
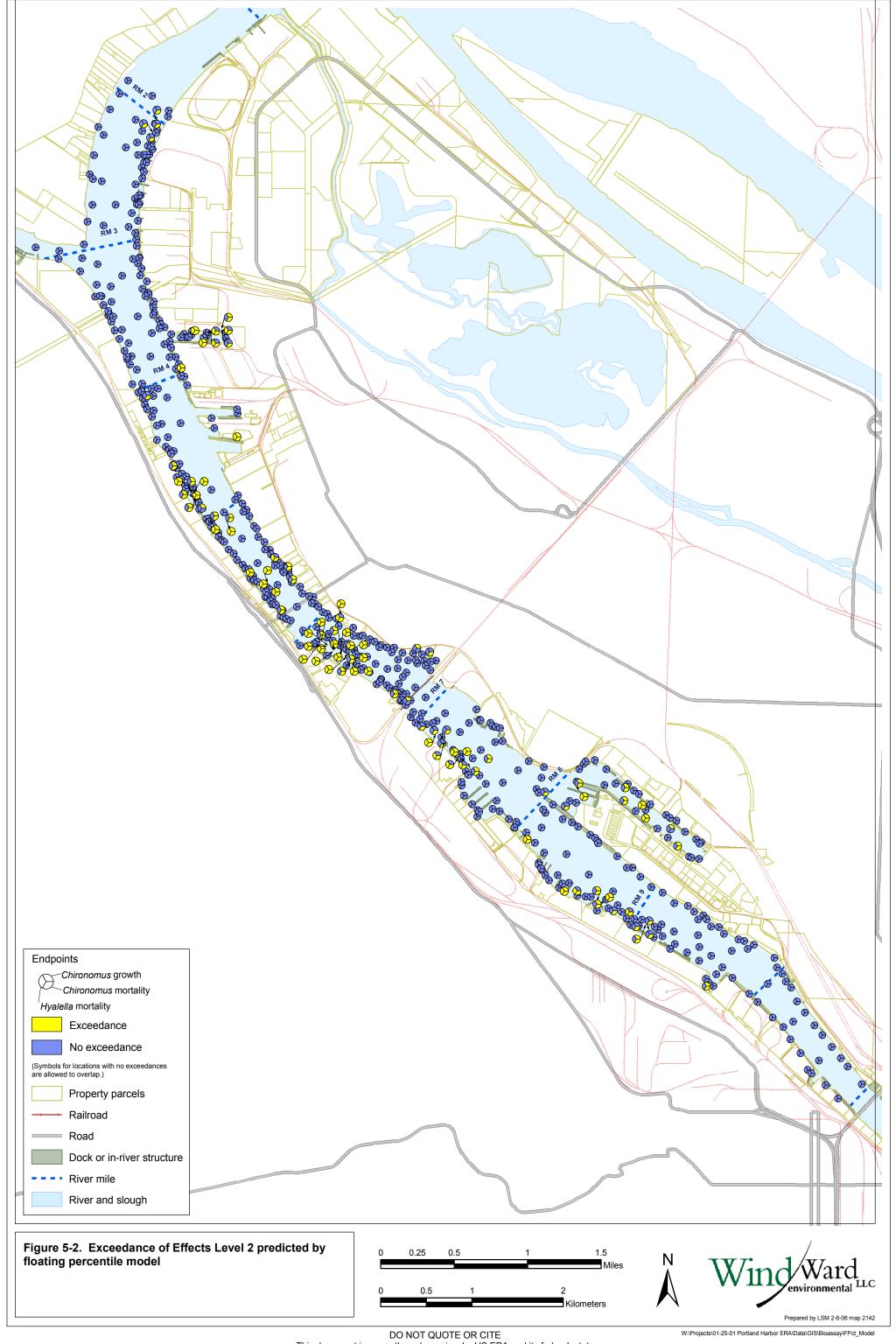
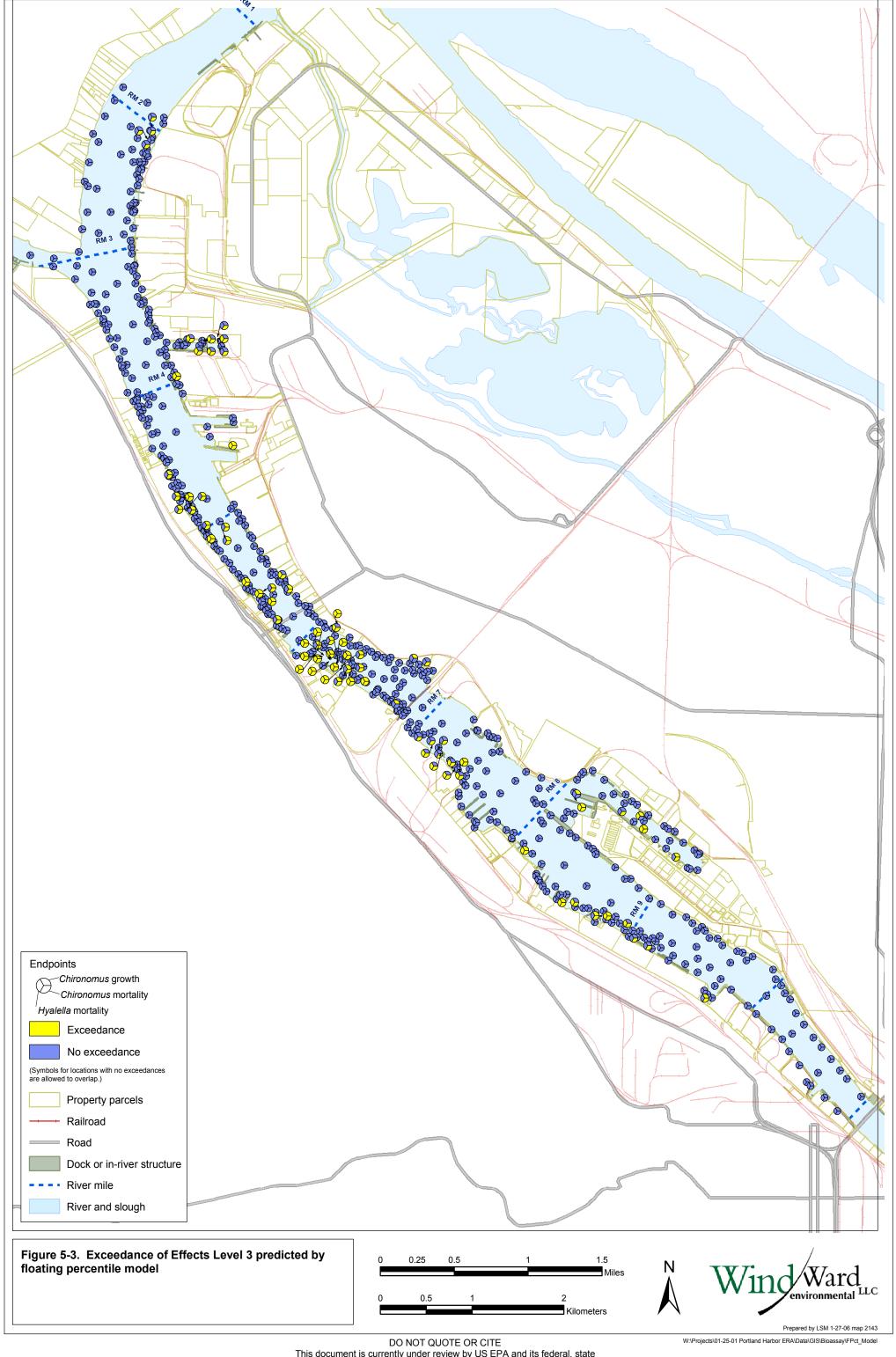
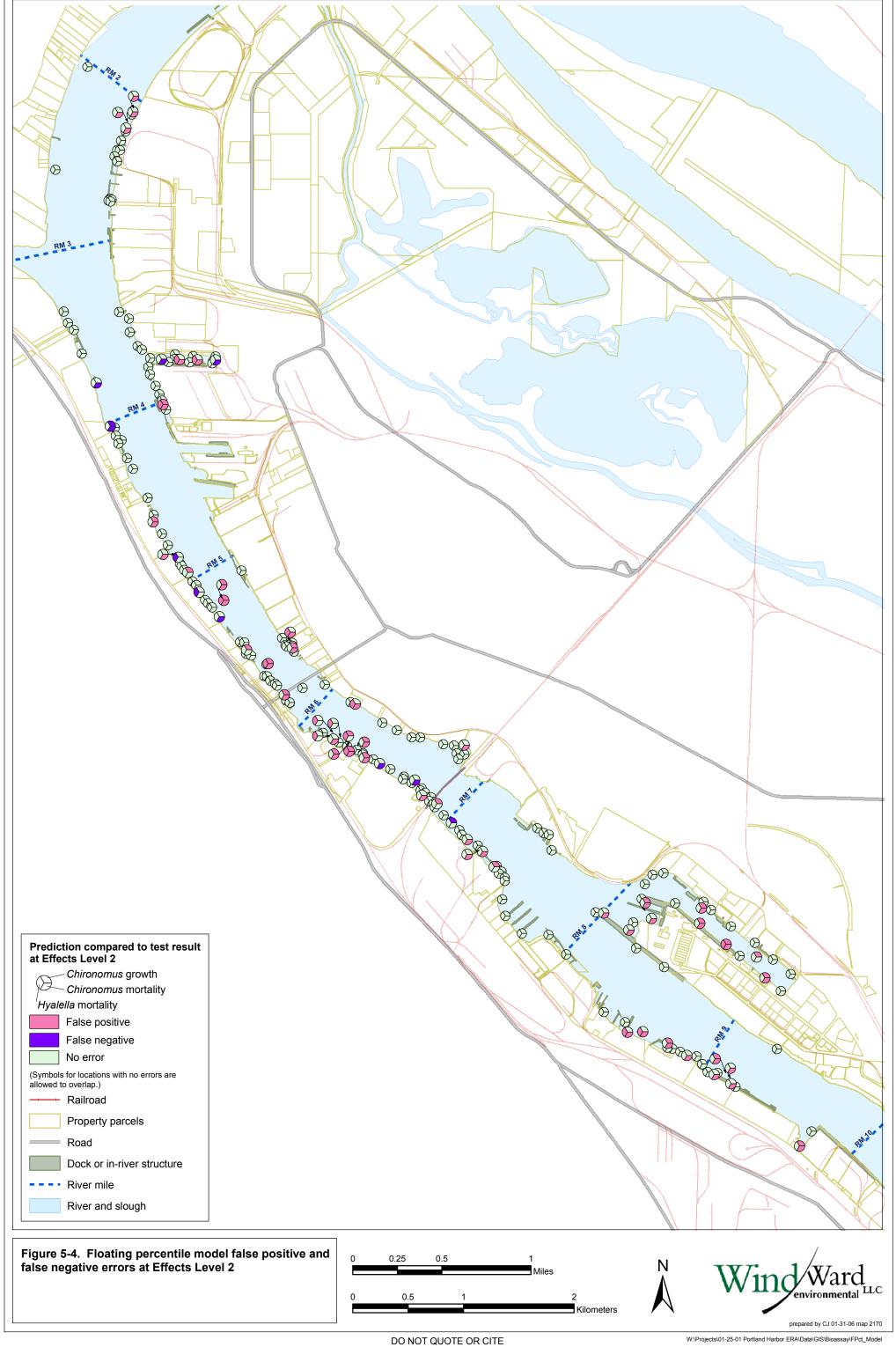
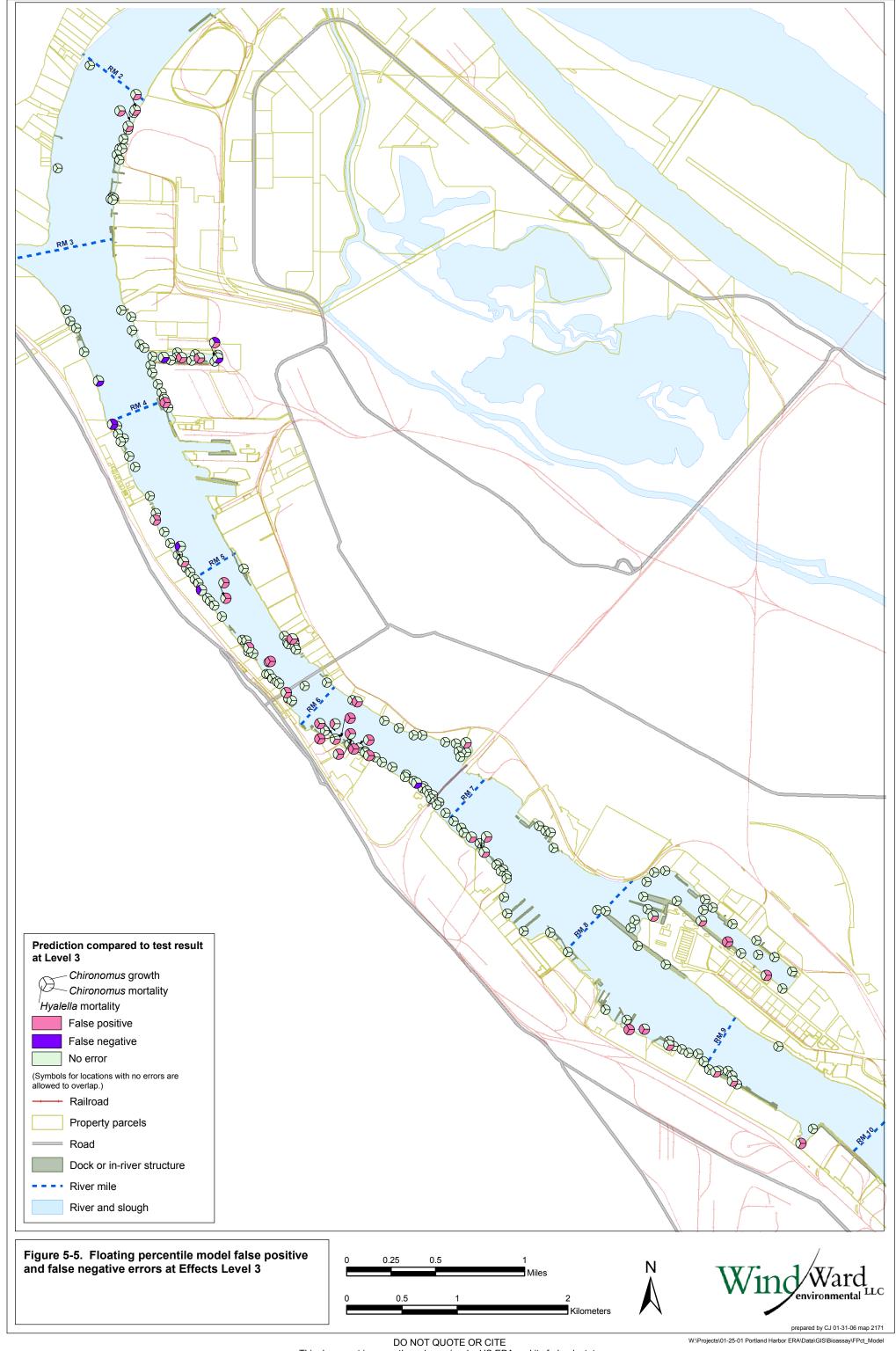


Figure 5-1. Floating percentile model









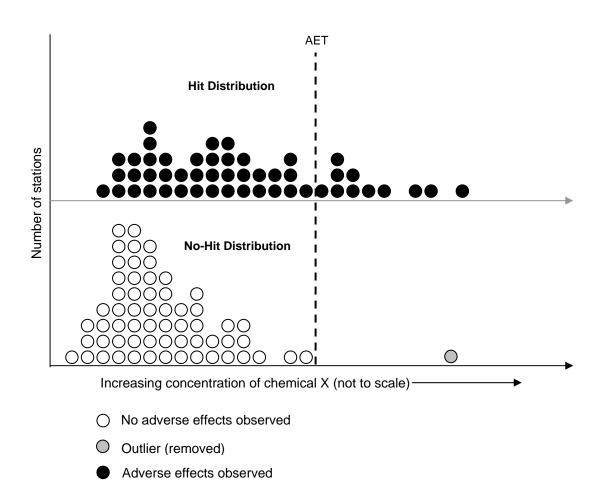


Figure 5-6. Calculation of apparent effects thresholds

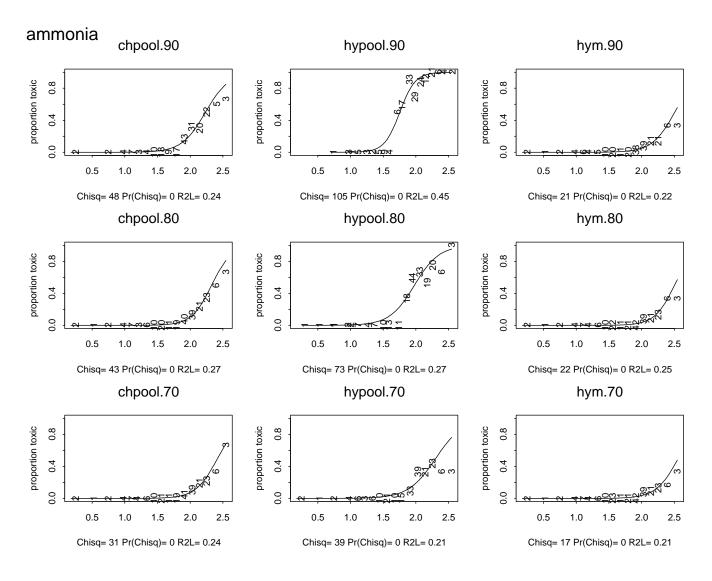


Figure 5-7. Individual logistic regression models for ammonia for three biological endpoints at three effects levels

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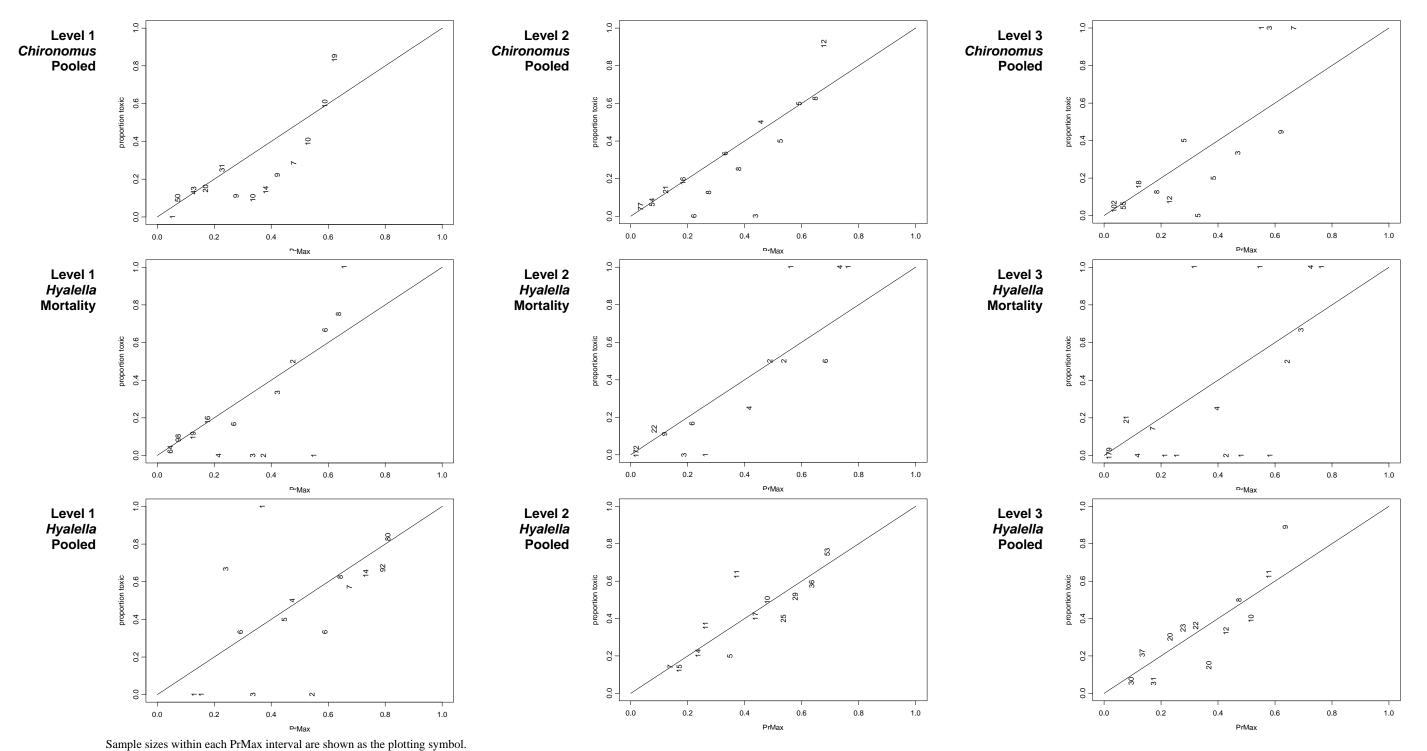
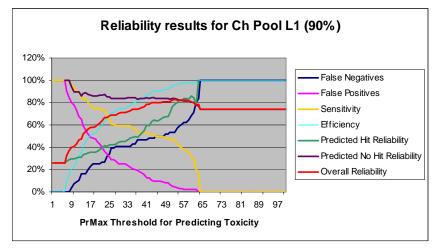
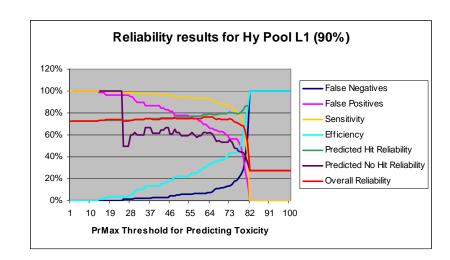
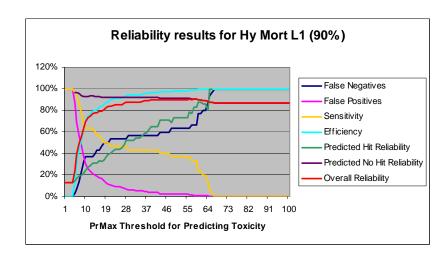
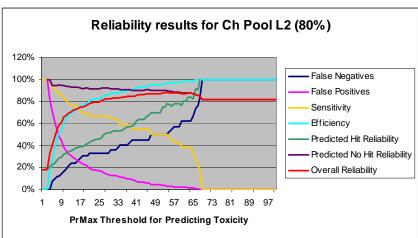


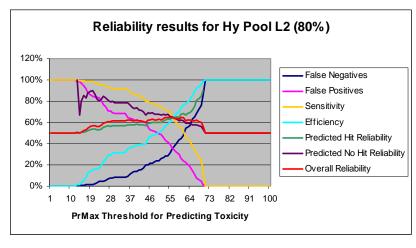
Figure 5-8. Median PrMax value and observed proportion of toxic data within PrMax intervals of 0.05

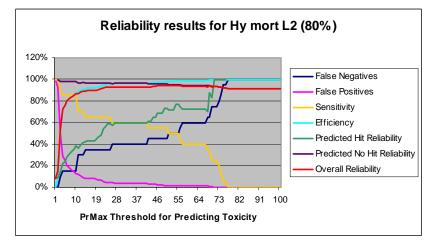


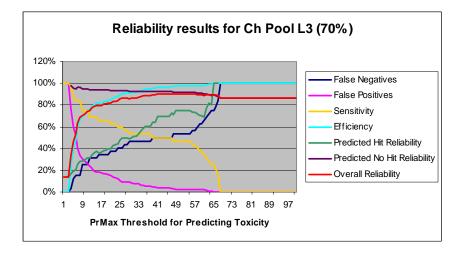


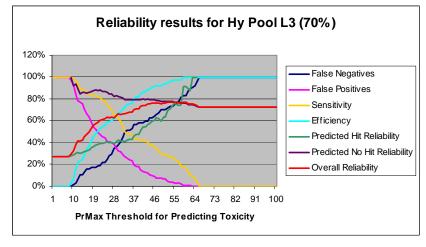












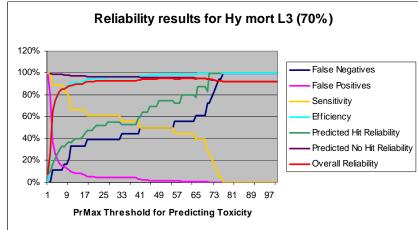


Figure 5-9. Reliability results for three biological endpoints at three effects levels

